

Newsletter 7 / 2021

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Save the date

Advanced C++ Course organised by CSCS: Oct. 11-13, 2021 (probably virtual).

Spread the word

Places available for the ESIWACE2 summer school on 23 to 27 August, 2021!

The registration for the [2021 Summer School on Effective HPC for Climate and Weather](#) is currently open!



Making effective use of HPC environments becomes increasingly challenging for PhD students and young researchers. As their primary intent is to generate insight, they often struggle with the technical nature of the tools and environments that enable their computer-aided research: computation, integration, and analysis of relevant data.

The scope of the summer school is the training of young researchers and software engineers in methods, tools, and theoretical knowledge to make effective use of HPC environments and generate insights. The school is supported by experts from international institutions that will be providing lectures and hands-on training in their field of expertise.

Date: 23-27 August, 2021

Venue: Virtual event

Deadline for registration: 31 July, 2021

Contact: Dr. Julian Kunkel <kunkel@hps.vi4io.org>

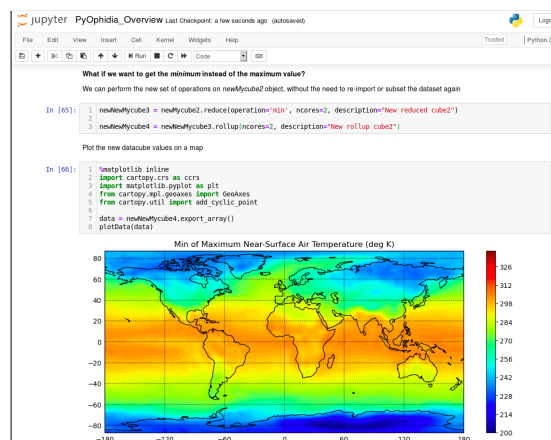
Further information:

<https://hps.vi4io.org/events/2021/esiwace-school>

Online training on High Performance Data Analytics and Visualisation from 13 to 16 September, 2021

This online training course provides an introduction to data analysis and visualisation applied to climate and weather domains, using high-performance data analytics and visualisation tools available from the open source market (i.e., Ophidia and ParaView).

The course is organised by CMCC and DKRZ in the context of the ESIWACE2 project and consists of four 2-hour online sessions held from the 13th to 16th of September, 2021. Each session combines presentations about the various topics and practical tutorials/hands-on. **The registration is open until 8 September, 2021.**



More information about the training event and the registration can be found at:

<https://www.esiwace.eu/events/hpda-vis-training-2021>

VECMA training event on EasySurrogate, QCG-PilotJob, and FabSim3

The VECMA project is offering a free online training on the VECMA software toolkit (VECMAtk), which establishes a platform for verification, validation and uncertainty quantification (VVUQ), with the goal of providing tools that can be combined to capture complex scenarios, applied to applications in disparate domains, and used to run multiscale simulations on any desktop, cluster or supercomputing platform. EasySurrogate is a new tool in the toolkit, aiming at surrogate modeling. To find out more and to register, please visit:

<https://www.vecma.eu/vecma-training-event-easysurrogate-qcg-pilotjob-and-fabsim3/>

Events that ESIWACE will participate in or has participated in

- [SC21](#), St. Louis, MO, USA, 14-19 November, 2021
- [Training on High Performance Data Analytics and Visualisation](#), online, 13-16 September, 2021
- [Summer School on effective HC for weather and climate](#), online, 23-27 August, 2021
- [PASC21](#), Geneva, Switzerland / online, 5-8 July, 2021
- [ISC 2021 High Performance Digital](#), online, 24 June - July 2, 2021
- [Teratec Forum 2021](#), online, 22-24 June, 2021
- [EGU General Assembly vEGU: Gather Online](#), online, 19-30 April, 2021

News & updates

9 people from around the world participated in the online course on “Code Coupling with OASIS3-MCT” from 29 April to May 12, 2021

A Small Private Online Course (SPOC) on OASIS3-MCT funded by ESIWACE2 was organised from April 29 to May 12 this year. 9 attendees from different countries around the world participated (France, Italy, UK, Germany, Spain, USA, Taiwan) in this training mixing theory, videos, quizzes and hands-on. The final survey indicates that the participants were quite pleased with the training, as 100% answered “yes” or “rather yes” to the questions on their general satisfaction. The next session is planned for early spring next year, so stay tuned!



More information on OASIS3-MCT is available on the [ESIWACE website](#) in the section on software support services.

New Atos blog post on improving weather and climate forecasting

In the new blog article, Erwan Raffin of Atos Bull explains why collaboration between domain scientists and High-Performance Computing experts is key for improving weather and climate forecasting. Read the full article at: <https://atos.net/en/blog/improving-weather-and-climate-forecasting-why-collaboration-between-domain-scientists-and-high-performance-computing-experts-is-key>

ESiWACE' Brexit - Waving goodbye to friends who are still around

By Reinhard Budich (RB) & Joachim Biercamp (JB)

It must have been 2001, I (RB) guess - my first time at the MetOffice, somewhere in a high-rise (ugly) building in downtown Exeter: One of the first meetings of PRISM, a project dealing with Software development for Earth System Modelling, initiated by the newly found European Network for Earth System Modeling: There I met

Mick Carter for the first time - and we laughed a lot at that meeting, as always, when Mick was around. With his superior in-depth knowledge about the workflows and processes involved in ESM, plus a profound knowledge of hard- and software problems, Mick always had smart ideas and surprising solutions to offer in any of our numerous meetings. So he was an asset to all the different projects we had the luck to participate in: PRISM, the different IS-ENES-n's, and a few others I have forgotten. Brussels was not a common home, but well-known turf, I claim.

Even longer ago, when year dates still started with a 19, **Mike Ashworth** had joined the German Climate Computing Center DKRZ, where he was one of the pioneers of parallelising climate codes. I (JB) still have a CD (!) from the Notting Hillbillies that Mike recommended to me and I will never forget the formidable genuine Christmas cake that he baked for us. In later years, back in the land of said cake, Mike was somehow always present in the community and contributed to the IS-ENES and ESIWACE projects in various ways.

Next on the list of Brexeteers is **Graham Riley** who joined together with Rupert Ford and was introduced to us as a specialist for Coding and Acceleration of Codes - and, boy, he delivered on that. Give him a piece of code, and he will return much better code.

Conclusion

So, ENES' / ESIWACE' Brexit? Kind of ... Who of the British long-time ENES fellows is still in? Bryan? No, he's a kiwi, Julian is German. Who else? Newbies will trundle in, we (RB&JB) are sure, but at least Rupert will hopefully stay around to keep the English humor up in the ENES projects!

Snapshots

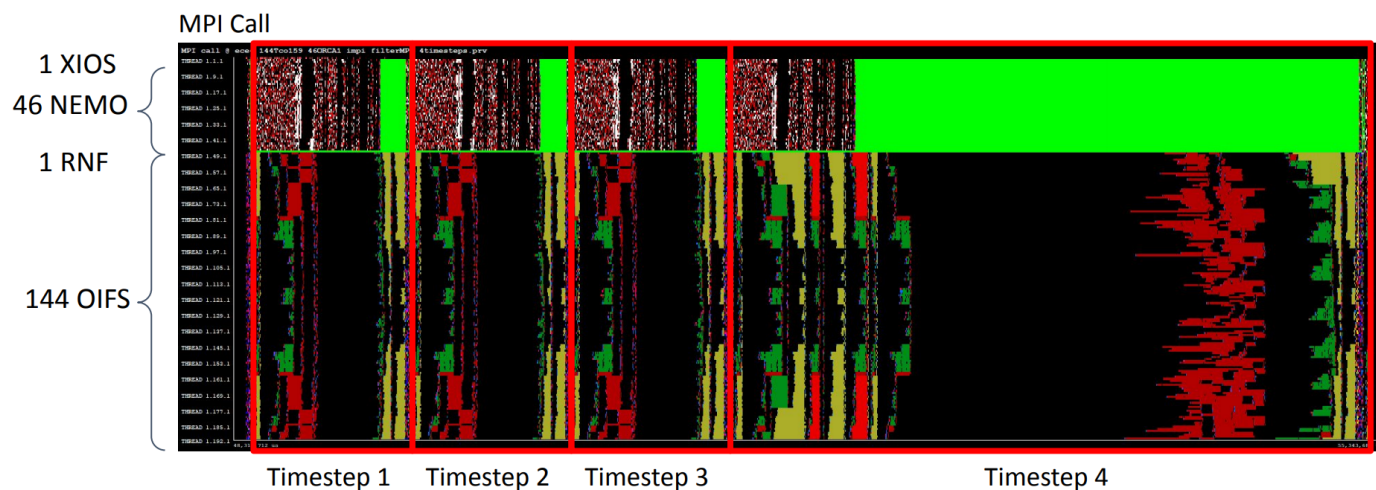
Atos Bull

Atos Bull is currently working on HPC user-service projects AGRIF, FESOM2 and RTE+RRTMGP C++ in collaboration with NLeSC.

BSC

BSC completed the first computational analysis of a standard EC-Earth4 run. The analysis includes a scalability test and profiling exercise. This analysis will bring new computational insights of the updated components of the model (OpenIFS43r3, NEMO4) and the full I/O management by XIOS.

Traces: Overview



After cutting the trace to omit the initialization and finalization phases, this is the recurrent pattern of the main computation (timesteps).



Figure: Trace of an EC-Earth4 standard run showing MPI states (NEMO top, OpenIFS bottom).

CERFACS

CERFACS completed the Small Private Online Course (SPOC) on OASIS3-MCT with additional exercises and a new section on regridding, and supervised the session organised from April 29th to May 12th that gathered 9 participants from around the world.

CMCC

An intermediate version of the ESDM-PAV Runtime and Python client has been released. A technical report documenting the new release and related implementation activities is being prepared and will be uploaded to

Zenodo. Preliminary extensions to Ophidia to support in-flight analytics at data loading time via ESDM have also been developed. Finally, CMCC contributed to the deliverable D2.10 “Machine Learning Workshop” concerning the “Workshop on New Opportunities for ML and AI in Weather and Climate Modelling”, held during March, 2021.

DKRZ

We have contributed to [VEGU](#) and are currently working on further processing and archiving simulation data from the DYAMOND initiative, especially DYAMOND winter simulation data, as they keep coming in.

Jointly with MPI-M, we are setting up and running global coupled 2.5 km and 10 km resolution simulations with the ICON model. Complex demo visualisations of 3D data from high resolution coupled and atmosphere-only ICON model simulations are also in the making.

Behind the scenes, we are overhauling the ESIWACE project website and are organising this year’s annual project meeting, which will take place as a virtual event in the last week of September.

ECMWF

Our paper investigating the replacement of physical parametrisation schemes in the ECMWF model, the IFS, by neural network emulators has been accepted by JAMES. The second paper looking into the automatic construction of tangent-linear and adjoint models with help from these neural network emulators is under peer review, also for JAMES (see publication list below).

We have started to port select components of the IFS to the ARM-based supercomputer Fugaku, through our collaboration with RIKEN and Oxford University. We have performed initial tests using half precision to accelerate the spectral transform package of the IFS. Although using half precision is surprisingly effective from a numerical perspective, we are still working on obtaining a good speed-up, compared with double precision.

We are also testing the latest official release of NEMO 4.0, 4.0.6, with single precision.

ETH Zürich / CSCS

CSCS is finishing preparations for the “Advanced C++” course (Oct. 11-13, 2021), which will offer important tips for getting C++ applications to run optimally for HPC. We will add this to “Events” as soon as possible. ESIWACE has 12 guaranteed slots; please consider joining us (most likely virtually, TBD).

ICHEC

ICHEC is testing the ESDM middleware in a full-stack environment including integration with Debian netcdf 4.8 in containers. We are planning to test this with operational workflows over the next few months.

Mercator Ocean International

An allocation of 24M CPU hours has been obtained on Mare Nostrum 4 through the PRACE 22nd call. This work, called the Submesoscale-permitting World Ocean Project, started in April 2021. This allocation will allow 1) to test on the NEMO global 1/36° new NEMO features that will improve the HPC performances and 2) to perform a multi year hindcast, forced by the 1 hours ECMWF IFS dataset.

NLeSC

NLeSC is currently working on performance optimisations in both DALES and RTE+RRTMGP service projects. For DALES, we are working on a mixed-precision implementation that is twice as fast as the double precision version and produces acceptable results. For RTE+RRTMGP, we are currently auto-tuning the GPU functions in the CUDA port of the RTE-RRTMGP-CPP code. We have first improved the memory management which improved the performance of the GPU code by a factor of 2.6x. Performance optimisations and auto-tuning of the GPU kernels in the longwave and shortwave solvers have further improved the performance by a factor of 10x. We are preparing a release of the GPU code.

Seagate

Seagate is continuing to develop the community around Mero. Seagate is also developing the advanced features of Mero (Function shipping) that could be used by weather & climate communities leveraging Mero based storage. Further, Mero has changed name to “Motr” and its ecosystem components inclusive (such as S3 etc) is called CORTX. This is in line with rebranding post open sourcing.

SMHI

The development of the production-like EC-Earth4 configuration is progressing. The latest milestone is the automatic generation of OASIS auxiliary files, which allows, among other things, to easily change the OpenIFS resolution. SMHI has also provided an EC-Earth 4 tutorial for new users in the community.

UKRI/STFC

Support for transforming an access to a single element of an array to a single trip loop in PSyclone is progressing. This will allow more NEMO code to be translated to SIR, particularly for boundary computation. The PSyclone-generated GPU version of NEMO without sea-ice is now running on a single V100 at 2.2x a 16 core Skylake CPU. An ORCA12 configuration has been run on up to 144 V100s on Marconi and performance overheads have been identified. Work continues on improving multi-GPU performance and will also start focusing more on the sea-ice part.

University of Reading

We have completed the organisation of the summer school and are looking forward to a wonderful event in August.

Recent ESiWACE2-related Publications

D. Elia, S. Fiore and G. Aloisio, “Towards HPC and Big Data Analytics Convergence: Design and Experimental Evaluation of a HPDA Framework for eScience at Scale,” in IEEE Access, vol. 9, pp. 73307-73326, 2021, doi: 10.1109/ACCESS.2021.3079139.

M. Chantry, S. Hatfield, P. Dueben, I. Polichtchouk, T. Palmer, “Machine learning emulation of gravity wave drag in numerical weather forecasting”, accepted in the Journal for Advances in Modeling Earth Systems, <https://arxiv.org/abs/2101.08195>.

S. E. Hatfield, M. Chantry, P. D. Dueben, P. Lopez, A. J. Geer, T. N. Palmer, "Building tangent-linear and adjoint models for data assimilation with neural networks", under review in the Journal for Advances in Modeling Earth Systems, <https://www.essoar.org/doi/abs/10.1002/essoar.10506310.1>.



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